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Dear Bolko,

This is the second quarterly report of our project under the current Thin Film Partnership Program (Subcontract No. XXL-5-44205-12 to University of Nevada, Las Vegas: Characterization of the electronic and chemical structure at thin film solar cell interfaces). A brief summary and details of our activities are given below. This report is in fulfillment of the deliverable schedule of the subcontract statement of work (SOW).

Summary

This project is devoted to deriving the electronic structure of interfaces in Cu(In,Ga)(S,Se)_2 and CdTe thin film solar cells. By using a unique combination of spectroscopic methods (photoelectron spectroscopy, inverse photoemission, and X-ray absorption and emission spectroscopy) a comprehensive picture of the electronic (i.e., band alignment in the valence and conduction band) as well as the chemical structure can be painted. The work focuses on (a) deriving the bench mark picture for world-record cells, (b) analyze state-of-the-art cells from industrial processes, and (c) aid in the troubleshooting of cells with substandard performance.

In our recent beamtime at the Advanced Light Source, Lawrence Berkeley National Laboratory we collected first results with Cu(In,Ga)Se_2 samples prepared by NREL. Together with additional photoemission measurements a detailed picture of the chemical composition at several interfaces and surfaces of the device structure can be drawn. The setup for inverse photoemission at UNLV was commissioned and first spectra were recorded.

Detailed Description of the Activities:

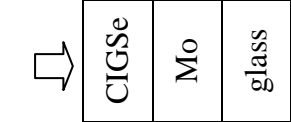
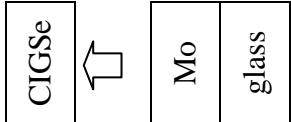
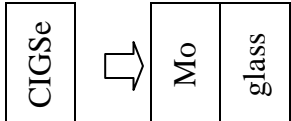
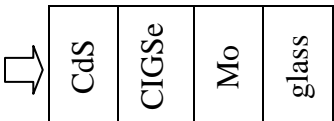
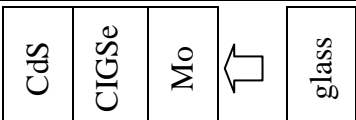
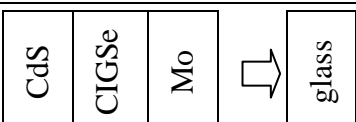
1. Investigation of Cu(In,Ga)Se_2 thin films from NREL

In our recent beamtime at the Advanced Light Source, Lawrence Berkeley National Laboratory from Nov. 2 – 13, 2005 we obtained first results with Cu(In,Ga)Se_2 (CIGSe) samples prepared by NREL. The investigations were based on two different samples, namely CIGSe/Mo/glass and CdS/CIGSe/Mo/glass. To investigate the interfaces buried beneath the absorber, namely the CIGSe/Mo interface and the Mo/glass interface, we

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have prepared additional samples by cleaving the samples at those interfaces. For doing so, we have glued the front side of both samples to stainless steel plates and cleaved the stack in two parts. For the CIGSe/Mo/glass sample, this cleavage takes place at the CIGSe/Mo-interface, as our measurements show. In contrast, the adhesion between the Mo back contact and the glass substrate was weak for the investigated CdS/CIGSe/Mo/glass sample (the reason for which is still under investigation), such that this sample cleaved at the Mo/glass interface. In total we thus investigated six different samples:

Table 1: List of investigated sample surfaces (the arrows show the direction of measurement).

Sample	Name in text	Schematic
CIGSe/Mo/glass	CIGSe front	
CIGSe/Mo/glass cleaved, top part	CIGSe back	
CIGSe/Mo/glass cleaved, bottom part	Mo front	
CdS/CIGSe/Mo/glass	CdS	
CdS/CIGSe/Mo/glass cleaved, top part	Mo back	
CdS/CIGSe/Mo/glass cleaved, bottom part	Glass front	

All samples were investigated by X-ray emission spectroscopy (XES) and the first three samples in Tab. 1 also by X-ray photoelectron spectroscopy (XPS). Both techniques provide detailed information about the chemical properties of the investigated samples and complement each other with respect to their surface sensitivity (XES: bulk-sensitive with an information depth of a few 100 nm; XPS: surface-sensitive with an information depth of a few nm).

Fig. 1 shows the XPS survey spectra of the CIGSe front, the CIGSe back, and the Mo front. The sample names in Tab. 1 are inspired by these surface-sensitive spectra, since Mo is only found on the “Mo front” sample and not on the “CIGSe back” sample.

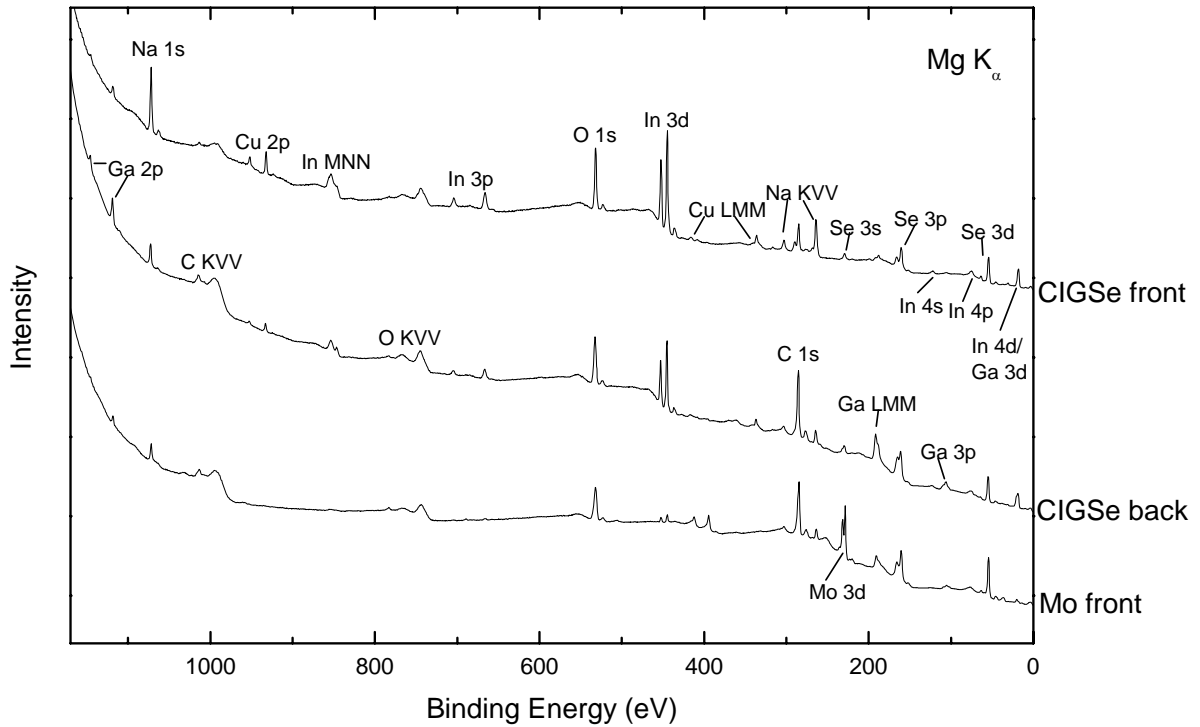


Fig. 1: XPS survey spectra of the CIGSe front, the CIGSe back and the Mo front of a $\text{Cu}(\text{In,Ga})\text{Se}_2$ absorber.

Since the samples were inevitably exposed to air prior to the measurements, a contamination layer consisting of C and O compounds is formed on their surface, complicating an exact quantitative analysis of the peak intensities. However, qualitative information can be gathered from the XPS survey spectra shown in Fig. 1.

We find that the In 3d signal is stronger on the CIGSe front than on the CIGSe back side. This is because a larger amount of indium is replaced by Ga at the absorber back, which can be seen from the stronger Ga 2p signal (compared to the absorber front).

The Na amounts on the three samples differ strongly. The highest Na content is found on the absorber front side, whereas much less Na is located around the CIGSe/Mo interface represented by the two other samples.

We find strong indications for different intermixing processes at the CIGSe/Mo interface, as will be discussed in the following. While only trace amounts of In and (within the detection limit of the experiment) no Cu is found, the Se signal increases at the Mo front, pointing towards the formation of a MoSe_2 compound, as was found before for $\text{Cu}(\text{In,Ga})(\text{S,Se})_2$ absorbers [1]. This finding is corroborated by the Mo $M_{4,5}$ XES spectra shown in Fig. 2. Here the $M_{4,5}$ emission of the Mo front is compared with that of the Mo back (note that the spectra of the CIGSe back and the glass front only show a small amount of residual Mo). In accordance with the assignment to MoSe_2 (with a smaller Mo density than in metal Mo), the Mo signal is significantly weaker at the Mo front (by a factor of 2.4).

In addition to the Se diffusion, a Ga diffusion into the Mo back contact can also be observed, which is manifested in the Ga 2p signal seen in the XPS survey spectrum of the Mo front in Fig. 1. The more bulk-sensitive XES measurements (mean free path of around 200 nm for photon energies around 1000 eV) in Fig. 3, where the Cu $L_{2,3}$, Na K, and Ga $L_{2,3}$ emission was recorded in one energy window, show that this Ga diffusion is

2. Commissioning of the setup for inverse photoemission (IPES)

The installation of the setup for IPES has been successfully completed and first spectra of an Ag reference sample were recorded. Those spectra are used for a calibration of the absolute energy scale of the setup, for which the position of the Fermi energy is measured. Fig. 4 shows the Fermi edge of the Ag conduction band measured with our setup (open circles). The red line represents a fit of the spectrum which is used to derive the Fermi energy, and, in addition, gives us the total energy resolution. We achieve a rather good total energy resolution of 440 meV, even though our setup is not yet optimized.

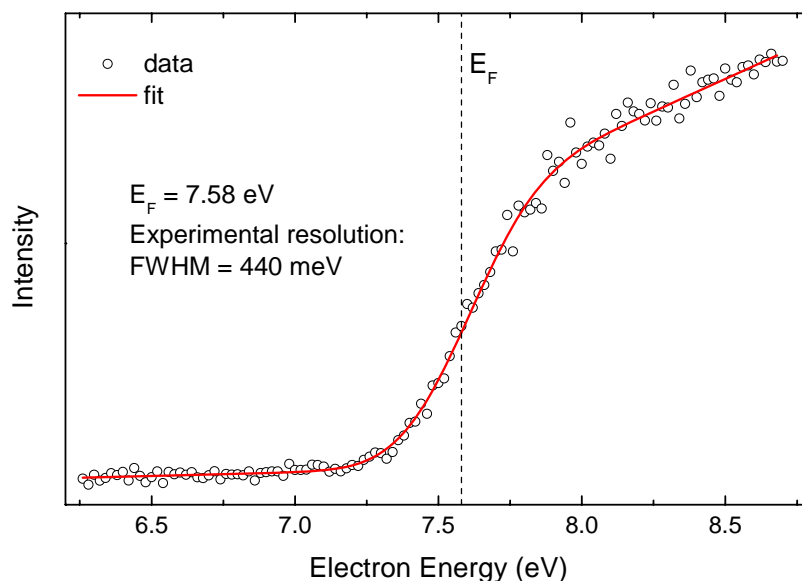


Fig. 4: Inverse photoemission (IPES) spectrum of an Ag reference sample (open circles). The red line represents a fit of the experimental data. The derived Fermi energy is given by the dashed vertical line.

- [1] L. Weinhardt, O. Fuchs, A. Peter, E. Umbach, C. Heske, J. Reichardt, M. Bär, I. Lauermann, I. Kötschau, A. Grimm, S. Sokoll, T.P. Niesen, S. Visbeck, and F. Karg, *J. Chem. Phys.*, in print (2006).
- [2] C. Heske, D. Eich, R. Fink, E. Umbach, T. van Buuren, C. Bostedt, S. Kakar, L. J. Terminello, M. M. Grush, T. A. Callcott, F. J. Himpsel, D. L. Ederer, R. C. C. Perera, W. Riedl, and F. Karg, *Surf. Interface Anal.* **30**, 459 (2000).

If you have any questions, please do not hesitate to call me at (702) 895-2694.

Sincerely,

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